Welcome to STN International! Enter x:x

LOGINID:ssspta1600rxa

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Apr 08	"Ask CAS" for self-help around the clock
NEWS 3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4	Apr 09	ZDB will be removed from STN
NEWS 5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 9	Jun 03	New e-mail delivery for search results now available
NEWS 10	Jun 10	MEDLINE Reload
NEWS 11	Jun 10	PCTFULL has been reloaded
NEWS 12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS 13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS 14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS 15	Jul 30	NETFIRST to be removed from STN
NEWS 16	Aug 08	CANCERLIT reload
NEWS 17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18	Aug 08	NTIS has been reloaded and enhanced
NEWS 19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS 20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS 23	Sep 03	JAPIO has been reloaded and enhanced
NEWS 24	Sep 16	Experimental properties added to the REGISTRY file
NEWS 25	Sep 16	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS 27	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS 28	Oct 21	EVENTLINE has been reloaded
NEWS 29	Oct 24	BEILSTEIN adds new search fields
NEWS 30	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 31	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS 32	Nov 18	DKILIT has been renamed APOLLIT
NEWS 33	Nov 25	More calculated properties added to REGISTRY
NEWS 34	Dec 02	TIBKAT will be removed from STN
NEWS 35	Dec 04	CSA files on STN

NEWS EXPRESS	October 14 CURRENT WINDOWS VERSION IS V6.01, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that

specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:09:53 ON 16 DEC 2002

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:10:00 ON 16 DEC 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 DEC 2002 HIGHEST RN 476300-36-4
DICTIONARY FILE UPDATES: 15 DEC 2002 HIGHEST RN 476300-36-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

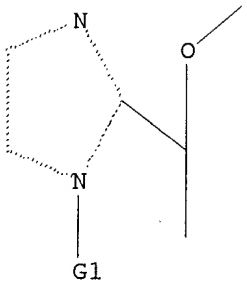
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09862808.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Cy———Ak[1]
G1 H,[@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:14:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 327 TO ITERATE

100.0% PROCESSED 327 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5456 TO 7624
PROJECTED ANSWERS: 6 TO 265

L2 6 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 09:14:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6459 TO ITERATE

100.0% PROCESSED 6459 ITERATIONS 168 ANSWERS
SEARCH TIME: 00.00.01

L3 168 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 142.94 143.15

FILE 'CAPLUS' ENTERED AT 09:14:36 ON 16 DEC 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 16 Dec 2002 VOL 137 ISS 25
FILE LAST UPDATED: 15 Dec 2002 (20021215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l3
L4 65 L3

=> s l3/p
L5 59 L3/P

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.79	143.94

FILE 'REGISTRY' ENTERED AT 09:15:32 ON 16 DEC 2002

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 DEC 2002 HIGHEST RN 476300-36-4
DICTIONARY FILE UPDATES: 15 DEC 2002 HIGHEST RN 476300-36-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

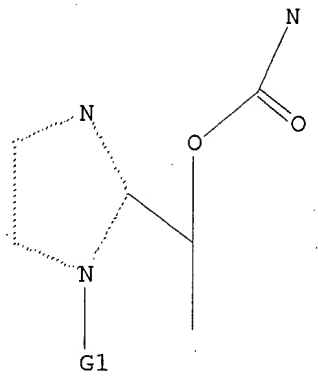
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading 09862808.str

L6 STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6 STR



Cy———Ak[1]
G1 H,[@1]

Structure attributes must be viewed using STN Express query preparation.

=> s l6
SAMPLE SEARCH INITIATED 09:15:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 16 TO ITERATE

100.0% PROCESSED 16 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 80 TO 560
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> s l6 full
FULL SEARCH INITIATED 09:15:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 350 TO ITERATE

100.0% PROCESSED 350 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L8 14 SEA SSS FUL L6

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	140.28	284.22

FILE 'CAPLUS' ENTERED AT 09:15:55 ON 16 DEC 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 16 Dec 2002 VOL 137 ISS 25
FILE LAST UPDATED: 15 Dec 2002 (20021215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s l8
L9 5 L8

=> d ibib abs hitstr 1-5

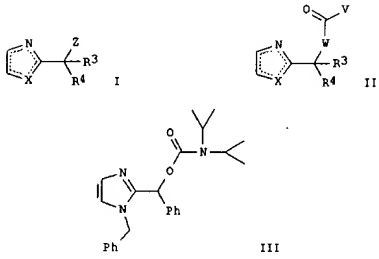
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:904116 CAPLUS
DOCUMENT NUMBER: 136:37606
TITLE: Synthesis of 2-substituted azoles via multicomponent reactions.
INVENTOR(S): Hlasta, Dennis
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094318	A2	20011213	WO 2001-US16727	20010522
WO 2001094318	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002042520	A1	20020411	US 2001-862808	20010522

PRIORITY APPLN. INFO.: US 2000-209252P P 20000605
OTHER SOURCE(S): CASREACT 136:37606; MARPAT 136:37606
GI

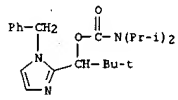


AB Title compds. [I; X = NH, NRa, S; Z = ORa, NRaRb, SR, cyano, N3, etc.; R3 = H, alkyl, (substituted) aralkyl, cycloalkyl, fluoroalkyl, COR, CO2R, etc.; R4 = alkyl, aryl, aralkyl, cycloalkyl, fluoroalkyl, alkenyl,

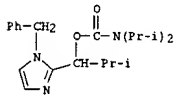
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)
alkynyl, COR, etc.; Ra, Rb = H, R, CO2R, COR, SO2R, SOR, etc.; R = alkyl, (substituted) aralkyl, cycloalkyl, adamantyl, norbornyl, fluoroalkyl, heterocyclyl], were prepd. by treatment of the corresponding unsubstituted azoles with ACOV (A = F, Cl, Br, OCOCMe3; V = sterically hindered group) and then with R3C(:W)R4 (W = O, NSO2R, NSOR, NCOR, NCO2R, NR; R as above) to give compds. (II; variables as above) followed by optional treatment of II with ZH (Z as above). Thus, 1-benzylimidazole in MeCN at 0.degree. was treated sequentially with diisopropylcarbamoyl chloride in MeCN, PhCHO, and diisopropylethylamine followed by 24 h reflux to give 78% title compd. (III).

IT **327626-33-5P 327626-34-6P 327626-35-7P**
327626-36-8P 327626-40-4P 327626-41-5P
327626-42-6P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-substituted azoles via multicomponent reactions)

RN 327626-33-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2-dimethyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

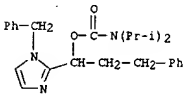


RN 327626-34-6 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-methyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

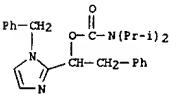


RN 327626-35-7 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 3-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

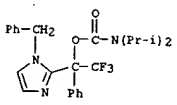
L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



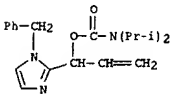
RN 327626-36-8 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 327626-40-4 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)

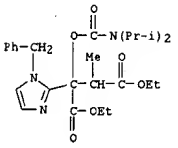


RN 327626-41-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 1-[1-(phenylmethyl)-1H-imidazol-2-yl]-2-propenyl ester (9CI) (CA INDEX NAME)

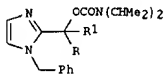


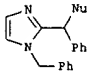
RN 327626-42-6 CAPLUS
CN Butanedioic acid, 2-[[[bis(1-methylethyl)amino]carbonyl]oxy]-3-methyl-2-[1-(phenylmethyl)-1H-imidazol-2-yl]-, diethyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:910341 CAPLUS
DOCUMENT NUMBER: 134:193376
TITLE: Novel use of imidazolium ylides in an efficient synthesis of 2-substituted imidazoles
AUTHOR(S): Hlasta, Dennis J.
CORPORATE SOURCE: Drug Discovery The R.W. Johnson Pharmaceutical Research Institute, Spring House, PA, 19477-0776, USA
SOURCE: Organic Letters (2001), 3(2), 157-159
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:193376
GI

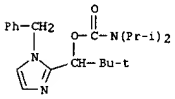

I


II

AB A new reaction of imidazoles was discovered involving the formation of an imidazolium ylide, which on trapping with various electrophiles afforded diverse 2-substituted imidazoles I (R = CMe3, R1 = H; R = Ph, R1 = H; R = Ph, R1 = CF3; etc.). The facile, convenient reaction conditions when compared to the existing procedures make this reaction the method of choice in the prepn. of 2-substituted imidazoles. Moreover, the reaction differs from the reported methods since the products contain an .alpha.-substituent that is transformed by solvolysis chem. into further functionalized derivs. II (Nu = H, MeO, EtO, etc.).

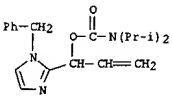
IT **327626-33-5P 327626-34-6P 327626-35-7P**
327626-36-8P 327626-40-4P 327626-41-5P
327626-42-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of imidazole derivs. by alkylation of imidazolium ylides)

RN 327626-33-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2-dimethyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

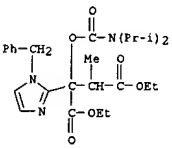


RN 327626-34-6 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-methyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)

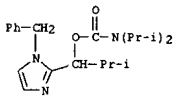


RN 327626-42-6 CAPLUS
CN Butanedioic acid, 2-[[[bis(1-methylethyl)amino]carbonyl]oxy]-3-methyl-2-[1-(phenylmethyl)-1H-imidazol-2-yl]-, diethyl ester (9CI) (CA INDEX NAME)

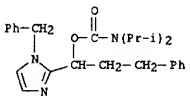


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

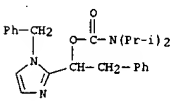
L9 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



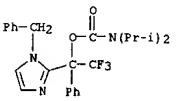
RN 327626-35-7 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 3-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)



RN 327626-36-8 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 327626-40-4 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)

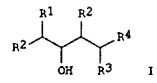


RN 327626-41-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 1-[1-(phenylmethyl)-1H-imidazol-2-yl]-2-propenyl ester (9CI) (CA INDEX NAME)

L9 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:207292 CAPLUS
DOCUMENT NUMBER: 128:270871
TITLE: Preparation of azolyl dipeptide analogs as retroviral protease inhibitors
INVENTOR(S): Carr, Thomas Joseph; Demarsh, Peter Lawrence; Dreyer, Geoffrey Bainbridge; Fenwick, Ashley Edward
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: U.S., 42 pp., Cont. of U.S. Ser. No. 193.026, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5733882	A	19980331	US 1995-396356	19950228
PRIORITY APPLN. INFO.:			US 1994-193026	19940117

OTHER SOURCE(S): MARPAT 128:270871
GI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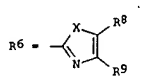

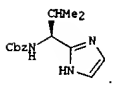
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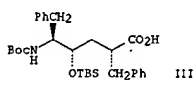
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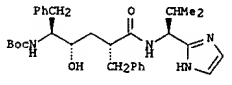

IV

AB The present invention provides compds., more particularly dipeptide analogs I [R1, R3 = independently (un)substituted Q, Q-C1-6 alkyl, Q-C2-6 alkenyl, Q-C2-6 alkynyl, C1-6 alkyl substituted by 1-5 F atoms; Q = H, C3-6 cycloalkyl, C5-6 cycloalkenyl, aryl, heterocyclyl; R2 = H, OH; R4 = R6NR11, CONR11CHR6R7; R5 = R6NR11, R10NR11; X = NR11, O, S; R7 = Q, Q-C1-6 alkyl, Q-C2-6 alkenyl; R8, R9 = independently H, OH, halo, NO2, acyl, CF3, aryl, etc.; R8R9 = fused C2-4 alkylene, aryl, heterocyclyl; R10 = A-(B)n; R11 = H, C1-4 alkyl; B = amino acid; A = H, (un)substituted aryl, heterocyclyl, aryl-W, heterocyclyl-W, phthaloyl, etc.; W = CO, O2C, NR11CO, SCO, NR11CS, SO2, NR11SO2, P(O)(OR22); R22 = H, C1-6 alkyl, Ph, phenyl-C1-4 alkyl; with provisos], or a pharmaceutically acceptable salt

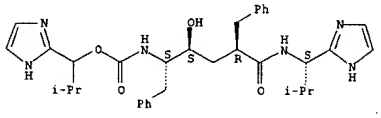
L9 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)
thereof, which bind to retroviral proteases. These compds. are inhibitors of retroviral proteases and are useful for treating diseases related to infection by retroviruses. Thus, cyclocondensation of protected valinal Z-Val-H (Z = PhCH2OC) with ammonia and glyoxal gave imidazole II. Deprotection of II, followed by coupling with dipeptide isostere III, and final desilylation gave desired title compd. IV as its HCl salt. The prepd. compds., including IV, showed inhibition of HIV-1 protease with Ki = 1 nM to 5 .mu.M, and inhibited infection of cells with the HIV virus with IC50 = 0.1 to 10 .mu.M.

IT **205595-86-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of azolyl dipeptide analogs as retroviral protease inhibitors)

RN 205595-86-4 CAPLUS

CN Carbamic acid, [2-hydroxy-5-[[1-(1H-imidazol-2-yl)-2-methylpropyl]amino]-5-oxo-1,4-bis(phenylmethyl)pentyl]-, 1-(1H-imidazol-2-yl)-2-methylpropyl ester, [1S-[1R*,2R*,4S*,5(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:517245 CAPLUS
DOCUMENT NUMBER: 119:117245
TITLE: Preparation of N-imidazolylalkyl-5-amino-4-hydroxyhexanamides and analogs as retroviral protease inhibitors
INVENTOR(S): Carr, Thomas Joseph; DeMarsh, Peter Lawrence; Penwick, Ashley Edward
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA
SOURCE: PCT Int. Appl., 146 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9302057	A1	19930204	WO 1992-US6047	19920717
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KR, LU, NL, NO, PL, RO, RU, SE, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
AU 9224129	A1	19930223	AU 1992-24129	19920717
CN 1071434	A	19930428	CN 1992-109761	19920717
ZA 9205360	A	19930614	ZA 1992-5360	19920717
EP 602069	A1	19940622	EP 1992-917238	19920717
R: BE, CH, DE, FR, GB, IT, LI, NL				
JP 07500577	T2	19950119	JP 1992-503016	19920717
ES 2068739	B1	19951101	ES 1993-107	19930121
ES 2068739	A1	19950416		

PRIORITY APPLN. INFO.: US 1991-731563 19910717
US 1992-870975 19920420
WO 1992-US6047 19920717

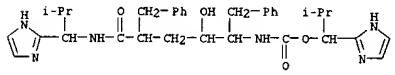
OTHER SOURCE(S): MARPAT 119:117245

AB R5CHR1CH(OH)CHR2CHR3R4 [I; R1, R3 = fluoroalkyl, cycloalk(en)yl(alkyl), aryl(alkyl), heterocyclyl(alkyl), etc.; R2 = H, OH; R4 = azolylamino, N-(azolylalkyl)carbamoyl; R5 = substituted amino] were prepd. Thus, Me2CHCHRNH2 (R = imidazol-2-yl) (prepn. given) was condensed with (2R, 4S, 5S)-PhCH2CH(NHCO2CMe3)CH(OR6)CH2CH(CH2Ph)COR7 (II; R6 = SiMe2CMe3, R7 = OH) to give, after deprotection, II (R6 = H, R7 = NHCHRCHMe2, R = imidazol-2-yl). I had Ki of 1 nM to 5 .mu.M for inhibition of HIV-1 protease.

IT **149356-57-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as retroviral protease inhibitor)

RN 149356-57-0 CAPLUS

CN Carbamic acid, [2-hydroxy-5-[[1-(1H-imidazol-2-yl)-2-methylpropyl]amino]-5-oxo-1,4-bis(phenylmethyl)pentyl]-, 1-(1H-imidazol-2-yl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



L9 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)

L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1968:78285 CAPLUS
DOCUMENT NUMBER: 68:78285
TITLE: Carbamates of 2-(hydroxyalkyl)benzimidazoles
INVENTOR(S): Bywater, William G.; Brown, Bernard Beau; Clegg, John M.
PATENT ASSIGNEE(S): Penick, S. B., and Co.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

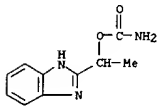
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3318889		19670509	US	19631014

GI For diagram(s), see printed CA Issue.

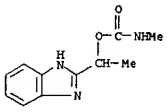
AB The title compds. (I) are prepd. by treatment of an o-phenylenediamine with an appropriate hydroxy carboxylic acid, and conversion of the hydroxyalkylbenzimidazole thus formed to the carbamate by standard methods. Thus, a mixt. of 0.5 mole 4,5-dichloro-o-phenylenediamine and 0.75 mole glycolic acid was refluxed for 4-6 hrs. in a soln. of 400 ml. concd. HCl and 400 ml. H2O to yield 82.3% 5,6-dichloro-2-hydroxymethylbenzimidazole (II), m. 270-1.degree. (decompn.) (MeOH). II(0.03 mole) was dissolved in 75 ml. dry pyridine at 70.degree., the soln. cooled to 40.degree. with stirring, 0.0475 mole Me isocyanate added, and the mixt. kept at 70.degree. for 30 min. to give 46% 5,6-dichloro-2-(N-methylcarbamoyloxymethyl)benzimidazole (III), m. 225.degree. (decompn.). Alternatively, 0.06 mole Me2NCOCl was added to 0.05 mole II dissolved in 150 ml. dry pyridine and the mixt. refluxed for 4 hrs. to give 45% 4,5-dichloro - 2 - (N,N - dimethylcarbamoyloxymethyl)benzimidazole (IV), m. 176-8.degree.. In another method, a mixt. consisting of 0.5 mole 2-(.alpha.-hydroxyethyl)benzimidazole, 0.55 mole urethane, and a catalytic amt. of (iso-PrO)3Al was refluxed in toluene for 32 hrs. during which time 5 addnl. 2-3-g. portions of (iso-PrO)3Al were added to give 11.5 g. 2-(.alpha.-carbamoyloxyethyl)benzimidazole (V), m. 207-7.5.degree.. Other I prepd. by these methods were: 5,6-dichloro-2-(.beta.-N-methylcarbamoyloxyethyl)benzimidazole, m. 147-53.degree. (decompn.); 5,6-dichloro-2-(.gamma.-N-methylcarbamoyloxypropyl)benzimidazole, m. 179-80.degree.; 5,6-dichloro-2-(N-ethylcarbamoyloxymethyl)benzimidazole (VI), m. 225-7.degree.; 5,6-dichloro-2-(.alpha.-N-methylcarbamoyloxybenzyl)benzimidazole (VII), m. 157-8.degree. (decompn.); 5,6-dichloro-2-(.alpha.-N-ethylcarbamoyloxybenzyl)-benzimidazole, m. 171-3.degree.; 2-(N-methylcarbamoyloxymethyl)-benzimidazole, m. 120-1.degree.; 2-(.alpha.-N-methylcarbamoyloxyethyl)-benzimidazole, m. 110-11.degree.; 5(6)-chloro-2-(N-methylcarbamoyloxymethyl)benzimidazole, m. 99-100.degree.; 5(6)-chloro-2-(.alpha.-N-methylcarbamoyloxyethyl)benzimidazole, m. 203-5.degree.; 5(6)-nitro-2(N-methylcarbamoyloxymethyl)benzimidazole, m. 199-201.degree.. Quaternizations of I were carried out as follows. Equimolar amts. of IV and 4-amino-5-bromomethyl-2-propylpyrimidine dihydrobromide (VIII) were dissolved in MeOH and an equal vol. of MeCN was added to give 50% 3-(4-amino-2-propyl-5-pyrimidinylmethyl) - 5,6 - dichloro - 2 - (N,N - dimethylcarbamoyloxymethyl)benzimidazolium bromide dihydrobromide, m. 270.degree. (charring). Quaternary salts were prepd. from VIII and the following I: V, VI, m. 170-5.degree. (decompn.), and VII. I are active against cecal coccidiosis in poultry and accelerate or retard certain sleep-inducing drugs.

IT **17577-51-4P 17577-58-1P 20258-42-6P**

L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)
28724-58-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 17577-51-4 CAPLUS
CN 2-Benzimidazolemethanol, .alpha.-methyl-, carbamate (ester) (8CI) (CA INDEX NAME)

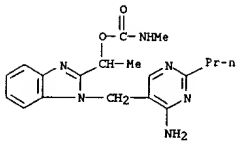


RN 17577-58-1 CAPLUS
CN Carbamic acid, methyl-, 1-(2-benzimidazolyl)ethyl ester (8CI) (CA INDEX NAME)



RN 28258-42-6 CAPLUS
CN Carbamic acid, methyl-, 1-[1-[(4-amino-2-propyl-5-pyrimidinyl)methyl]-5(or 6)-chloro-2-benzimidazolyl]ethyl ester, trihydrobromide (8CI) (CA INDEX NAME)

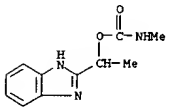
L9 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS (Continued)



D1—Cl

●3 HBr

RN 28724-58-5 CAPLUS
CN Carbamic acid, methyl-, 1-(5-chloro-2-benzimidazolyl)ethyl ester (8CI) (CA INDEX NAME)



D1—Cl

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FULL ESTIMATED COST	22.74	306.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.10	-3.10

FILE 'REGISTRY' ENTERED AT 09:17:19 ON 16 DEC 2002

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 DEC 2002 HIGHEST RN 476300-36-4
DICTIONARY FILE UPDATES: 15 DEC 2002 HIGHEST RN 476300-36-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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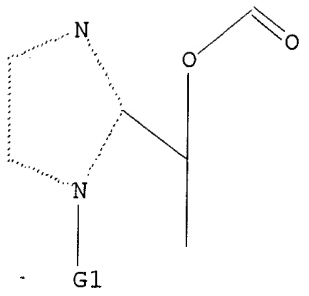
L10 HAS NO ANSWERS
L10 STR



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Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -    104 TO ITERATE

100.0% PROCESSED     104 ITERATIONS                          1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1469 TO     2691
PROJECTED ANSWERS:               1 TO       80

L11           1 SEA SSS SAM L10

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FULL SEARCH INITIATED 09:17:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1844 TO ITERATE

100.0% PROCESSED    1844 ITERATIONS                         62 ANSWERS
SEARCH TIME: 00.00.01

L12          62 SEA SSS FUL L10

=> fil caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.10

FILE 'CAPLUS' ENTERED AT 09:17:32 ON 16 DEC 2002

FILE COVERS 1907 - 16 Dec 2002 VOL 137 ISS 25
FILE LAST UPDATED: 15 Dec 2002 (20021215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

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L13 26 L12

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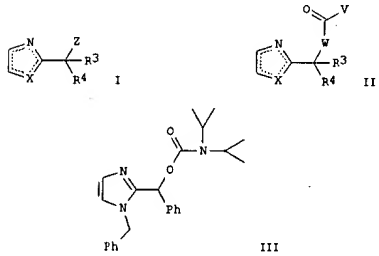
L13 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:904116 CAPLUS
DOCUMENT NUMBER: 136:37606
TITLE: Synthesis of 2-substituted azoles via multicomponent reactions.
INVENTOR(S): Hlasta, Dennis
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 80 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001094318	A2	20011213	WO 2001-US16727	20010522
WO 2001094318	A3	20020718		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002042520	A1	20020411	US 2001-862808	20010522

PRIORITY APPLN. INFO.: US 2000-209252P P 20000605
OTHER SOURCE(S): CASREACT 136:37606; MARPAT 136:37606
GI

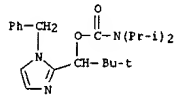


AB Title compds. [I; X = NH, NRa, S; Z = ORa, NRaRb, SR, cyano, N3, etc.; R3 = H, alkyl, (substituted) aralkyl, cycloalkyl, fluoroalkyl, COR, CO2R, etc.; R4 = alkyl, aryl, aralkyl, cycloalkyl, fluoroalkyl, alkenyl,

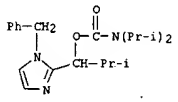
L13 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
alkynyl, COR, etc.; Ra, Rb = H, R, CO2R, COR, SO2R, SOR, etc.; R = alkyl, (substituted) aralkyl, cycloalkyl, adamantyl, norbornyl, fluoroalkyl, heterocyclyl], were prepd. by treatment of the corresponding unsubstituted azoles with ACOV (A = F, Cl, Br, OCOCMe3; V = sterically hindered group) and then with R3C(:W)R4 (W = O, NSO2R, NSOR, NCOR, NCO2R, NR; R as above) to give compds. (II; variables as above) followed by optional treatment of II with ZH (Z as above). Thus, 1-benzylimidazole in MeCN at 0.degree. was treated sequentially with diisopropylcarbamoyl chloride in MeCN, PhCHO, and diisopropylethylamine followed by 24 h reflux to give 78% title compd. (III).

IT **327626-33-5P 327626-34-6P 327626-35-7P**
327626-36-8P 327626-40-4P 327626-41-5P
327626-42-6P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 2-substituted azoles via multicomponent reactions)

RN 327626-33-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2-dimethyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

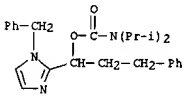


RN 327626-34-6 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-methyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

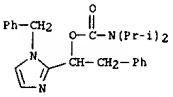


RN 327626-35-7 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 3-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

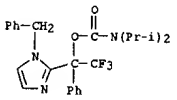
L13 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



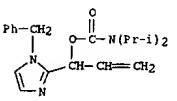
RN 327626-36-8 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 327626-40-4 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)

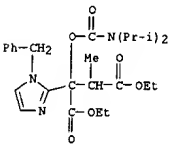


RN 327626-41-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 1-[1-(phenylmethyl)-1H-imidazol-2-yl]-2-propenyl ester (9CI) (CA INDEX NAME)

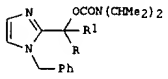


RN 327626-42-6 CAPLUS
CN Butanedioic acid, 2-[[[bis(1-methylethyl)amino]carbonyl]oxy]-3-methyl-2-[1-(phenylmethyl)-1H-imidazol-2-yl]-, diethyl ester (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



L13 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:910341 CAPLUS
DOCUMENT NUMBER: 134:193376
TITLE: Novel use of imidazolium ylides in an efficient synthesis of 2-substituted imidazoles
AUTHOR(S): Hlasta, Dennis J.
CORPORATE SOURCE: Drug Discovery The R.W. Johnson Pharmaceutical Research Institute, Spring House, PA, 19477-0776, USA
SOURCE: Organic Letters (2001), 3(2), 157-159
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:193376
GI



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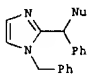
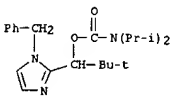


II

AB A new reaction of imidazoles was discovered involving the formation of an imidazolium ylide, which on trapping with various electrophiles afforded diverse 2-substituted imidazoles I (R = CMe3, R1 = H; R = Ph, R1 = H; R = Ph, R1 = CF3; etc.). The facile, convenient reaction conditions when compared to the existing procedures make this reaction the method of choice in the prepn. of 2-substituted imidazoles. Moreover, the reaction differs from the reported methods since the products contain an .alpha.-substituent that is transformed by solvolysis chem. into further functionalized derivs. II (Nu = H, MeO, EtO, etc.).

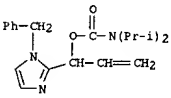
IT **327626-33-5P 327626-34-6P 327626-35-7P**
327626-36-8P 327626-40-4P 327626-41-5P
327626-42-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of imidazole derivs. by alkylation of imidazolium ylides)

RN 327626-33-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2-dimethyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

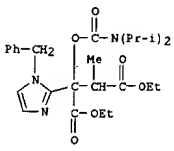


RN 327626-34-6 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-methyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)

L13 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)

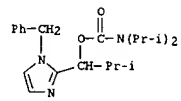


RN 327626-42-6 CAPLUS
CN Butanedioic acid, 2-[[[bis(1-methylethyl)amino]carbonyl]oxy]-3-methyl-2-[1-(phenylmethyl)-1H-imidazol-2-yl]-, diethyl ester (9CI) (CA INDEX NAME)

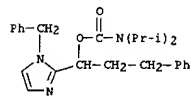


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

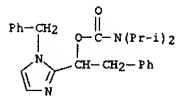
L13 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



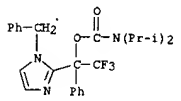
RN 327626-35-7 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 3-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]propyl ester (9CI) (CA INDEX NAME)



RN 327626-36-8 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 327626-40-4 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 2,2,2-trifluoro-1-phenyl-1-[1-(phenylmethyl)-1H-imidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



RN 327626-41-5 CAPLUS
CN Carbamic acid, bis(1-methylethyl)-, 1-[1-(phenylmethyl)-1H-imidazol-2-yl]-2-propenyl ester (9CI) (CA INDEX NAME)

L13 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:608618 CAPLUS
DOCUMENT NUMBER: 129:230735
TITLE: Preparation of cycloimido-substituted benzofused heterocyclic herbicides
INVENTOR(S): Crawford, Scott D.; Maravetz, Lester L.; Theodoridis, George; Dugan, Benjamin
PATENT ASSIGNEE(S): FMC Corp., USA
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9838188	A1	19980903	WO 1998-US3647	19980225
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6077812	A	20000620	US 1998-28636	19980224
ZA 9801580	A	19980827	ZA 1998-1580	19980225
AU 9866670	A1	19980918	AU 1998-66670	19980225
AU 734666	B2	20010621		
EP 968207	A1	20000105	EP 1998-908708	19980225
R: BE, CH, DE, ES, FR, GB, GR, IT, LI, NL				
BR 9807607	A	20000222	BR 1998-7607	19980225
JP 2002521001	T2	20020709	JP 1998-537797	19980225
US 6352958	B1	20020305	US 2000-547609	20000412

PRIORITY APPLN. INFO.: US 1997-39172P P 19970226
US 1998-28636 A 19980224
WO 1998-US3647 W 19980225

OTHER SOURCE(S): MARPAT 129:230735
GI

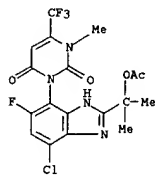
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; A, B = (un)substituted CH, N, (un)substituted NH, O; R = H, OH, SH, etc.; X = H, F, Cl, etc.; n = 0-3; J = II-VII (wherein R3 = H, alkyl, haloalkyl, etc.)], useful in controlling weeds, were prepd. Thus, heating at reflux 1-methyl-6-trifluoromethyl-3-(6-amino-4-bromo-2-fluoro-5-hydroxyphenyl)-2,4(1H,3H)-pyrimidinedione with carbonylimidazole in THF followed by reaction of the resulting 1-methyl-3-trifluoromethyl-3-(7-bromo-5-fluorobenzoxazol-2-on-4-yl)-2,4(1H,3H)-pyrimidinedione with MeI in the presence of Ag2O in CH2Cl2 afforded VIII which showed 100% control against, e.g., velvetleaf and blackgrass.

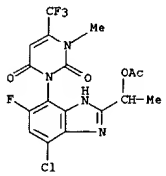
IT **212754-08-0P 212754-56-8P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of cycloimido-substituted benzofused heterocyclic herbicides)

RN 212754-08-0 CAPLUS

L13 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
CN 2,4(1H,3H)-Pyrimidinedione, 3-[2-[1-(acetyloxy)-1-methylethyl]-7-chloro-5-fluoro-1H-benzimidazol-4-yl]-1-methyl-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

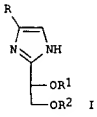


RN 212754-56-8 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione, 3-[2-(1-(acetyloxy)ethyl]-7-chloro-5-fluoro-1H-benzimidazol-4-yl]-1-methyl-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

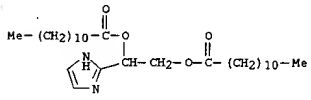


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:408105 CAPLUS
DOCUMENT NUMBER: 129:175592
TITLE: Synthesis of 1-(1H-imidazol-2-yl)ethane-1,2-diol derivatives. A novel class of protein kinase C inhibitors
AUTHOR(S): Roehrle, Andreas N.; Schmidhammer, Helmut
CORPORATE SOURCE: Inst. Pharmaceutical Chem., Univ. Innsbruck, Innsbruck, A-6020, Austria
SOURCE: Helvetica Chimica Acta (1998), 81(6), 1070-1076
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta AG
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:175592
GI

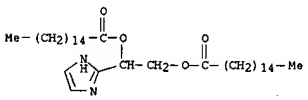


AB The title compds. I (R = H, Me; R1, R2 = Ac, dodecanoyl, hexadecanoyl, Me) were prepd. starting from appropriate 1-(triphenylmethyl)-protected 1H-imidazoles by lithiation with BuLi in THF followed by reaction with Ph3COCH2CHO, O-methylation, cleavage of N- and O-trityl protecting groups, and finally acylation. I (R = H, Me; R1 = R2 = dodecanoyl, hexadecanoyl) exhibited moderate protein kinase C inhibition.
IT **211488-57-2P 211488-58-3P 211488-60-7P**
211488-61-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of acylated (imidazolyl)ethanediols as protein kinase C inhibitors)
RN 211488-57-2 CAPLUS
CN Dodecanoic acid, 1-(1H-imidazol-2-yl)-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

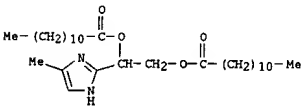


RN 211488-58-3 CAPLUS

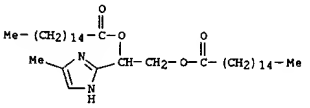
L13 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
CN Hexadecanoic acid, 1-(1H-imidazol-2-yl)-1,2-ethanediyl ester (9CI) (CA INDEX NAME)



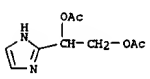
RN 211488-60-7 CAPLUS
CN Dodecanoic acid, 1-(4-methyl-1H-imidazol-2-yl)-1,2-ethanediyl ester (9CI) (CA INDEX NAME)



RN 211488-61-8 CAPLUS
CN Hexadecanoic acid, 1-(4-methyl-1H-imidazol-2-yl)-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

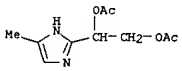


IT **211488-56-1P 211488-59-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of acylated (imidazolyl)ethanediols as protein kinase C inhibitors)
RN 211488-56-1 CAPLUS
CN 1,2-Ethanediol, 1-(1H-imidazol-2-yl)-, diacetate (ester) (9CI) (CA INDEX NAME)



RN 211488-59-4 CAPLUS
CN 1,2-Ethanediol, 1-(4-methyl-1H-imidazol-2-yl)-, diacetate (ester) (9CI) (CA INDEX NAME)

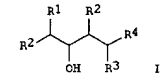
L13 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



L13 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:207292 CAPLUS
DOCUMENT NUMBER: 128:270871
TITLE: Preparation of azolyl dipeptide analogs as retroviral protease inhibitors
INVENTOR(S): Carr, Thomas Joseph; Demarsh, Peter Lawrence; Dreyer, Geoffrey Bainbridge; Fenwick, Ashley Edward
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: U.S., 42 pp., Cont. of U.S. Ser. No. 193.026, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5733882	A	19980331	US 1995-396356	19950228

PRIORITY APPLN. INFO.: US 1994-193026 19940117
OTHER SOURCE(S): MARPAT 128:270871
GI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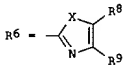
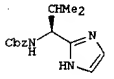
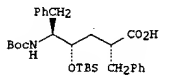
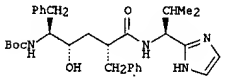



II

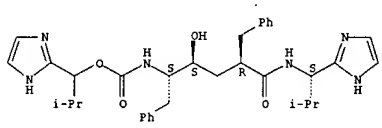

III


IV

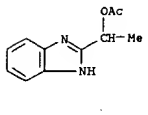
AB The present invention provides compds., more particularly dipeptide analogs I [R1, R3 = independently (un)substituted Q, Q-C1-6 alkyl, Q-C2-6 alkenyl, Q-C2-6 alkynyl, C1-6 alkyl substituted by 1-5 F atoms; Q = H, C3-6 cycloalkyl, C5-6 cycloalkenyl, aryl, heterocyclyl; R2 = H, OH; R4 = R6NR11, CONR11CHR6R7; R5 = R6NR11, R10NR11; X = NR11, O, S; R7 = Q, Q-C1-6 alkyl, Q-C2-6 alkenyl; R8, R9 = independently H, OH, halo, NO2, acyl, CF3, aryl, etc.; R8R9 = fused C2-4 alkylene, aryl, heterocyclyl; R10 = A-(B)n; R11 = H, C1-4 alkyl; B = amino acid; A = H, (un)substituted aryl, heterocyclyl, aryl-W, heterocyclyl-W, phthaloyl, etc.; W = CO, O2C,

L13 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
NR11CO, SCO, NR11CS, SO2, NR11SO2, P(O)(OR22); R22 = H, C1-6 alkyl, Ph, phenyl-C1-4 alkyl; with provisos], or a pharmaceutically acceptable salt thereof, which bind to retroviral proteases. These compds. are inhibitors of retroviral proteases and are useful for treating diseases related to infection by retroviruses. Thus, cyclocondensation of protected valinal Z-Val-H (Z = PhCH2O2C) with ammonia and glyoxal gave imidazole II. Deprotection of II, followed by coupling with dipeptide isostere III, and final desilylation gave desired title compd. IV as its HCl salt. The prepd. compds., including IV, showed inhibition of HIV-1 protease with Ki = 1 nM to 5 .mu.M, and inhibited infection of cells with the HIV virus with IC50 = 0.1 to 10 .mu.M.
IT **205595-86-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of azolyl dipeptide analogs as retroviral protease inhibitors)
RN 205595-86-4 CAPLUS
CN Carbamic acid, [2-hydroxy-5-[[1-(1H-imidazol-2-yl)-2-methylpropyl]amino]-5-oxo-1,4-bis(phenylmethyl)pentyl]-, 1-(1H-imidazol-2-yl)-2-methylpropyl ester, [1S-[1R*,2R*,4S*,5(R*)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



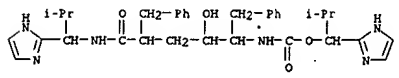
L13 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:652011 CAPLUS
DOCUMENT NUMBER: 125:328605
TITLE: 2-Alkyl substituted benzimidazole derivatives and their antifungal activities
AUTHOR(S): Gunes, H. Semih; Cosar, Guner
CORPORATE SOURCE: Faculty of Pharmacy, Ege University, Izmir, 35100, Turk.
SOURCE: Journal of Faculty of Pharmacy of Gazi University (1996), 13(1), 57-64
CODEN: JFPUE3; ISSN: 1015-9592
PUBLISHER: Gazi Universitesi, Eczacilik Fakultesi Dekanligi
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Different chem. procedures have been used for the synthesis of nine benzimidazole derivs. The compds. were tested for antifungal activity by the agar diln. method, using yeast-like fungi (Candida albicans 5405-11, Candida tropicalis 5401-11, Candida pseudotropicalis 164-12, Candida parapsilosis 768-2, Torulopsis glabrata 1434-1). 2-Methyl-1H-benzimidazole, 2-hydroxymethyl-1H-benzimidazole, 2-(1-hydroxyethyl)-1-H-benzimidazole, 2-(1-acetoxyethyl)-1H-benzimidazole, and 2-(1H-benzimidazol-2-yl)acetonitrile showed considerable activity against Candida tropicalis and weak activity against Torulopsis glabrata. QSAR studies have been performed using log P and log 1/C values.
IT **183244-70-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antifungal activity of benzimidazoles)
RN 183244-70-4 CAPLUS
CN 1H-Benzimidazole-2-methanol, .alpha.-methyl-, acetate (ester) (9CI) (CA INDEX NAME)



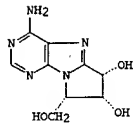
L13 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:517245 CAPLUS
DOCUMENT NUMBER: 119:117245
TITLE: Preparation of N-imidazolylalkyl-5-amino-4-hydroxyhexanamides and analogs as retroviral protease inhibitors
INVENTOR(S): Carr, Thomas Joseph; DeMarsh, Peter Lawrence; Penwick, Ashley Edward
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA
SOURCE: PCT Int. Appl., 146 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9302057	A1	19930204	WO 1992-US6047	19920717
W: AT, AU, BB, BG, BR, CA, CH, CS, DE, DK, ES, FI, GB, HU, JP, KR, LU, NL, NO, PL, RO, RU, SE, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
AU 9224129	A1	19930223	AU 1992-24129	19920717
CN 1071434	A	19930428	CN 1992-109761	19920717
ZA 9205360	A	19930614	ZA 1992-5360	19920717
EP 602069	A1	19940622	EP 1992-917238	19920717
R: BE, CH, DE, FR, GB, IT, LI, NL				
JP 07500577	T2	19950119	JP 1992-503016	19920717
ES 2068739	B1	19951101	ES 1993-107	19930121
ES 2068739	A1	19950416		

PRIORITY APPLN. INFO.: US 1991-731563 19910717
US 1992-870975 19920420
WO 1992-US6047 19920717
OTHER SOURCE(S): MARPAT 119:117245
AB R5CHR1CH(OH)CHR2CHR3R4 [I; R1, R3 = fluoroalkyl, cycloalk(en)yl(alkyl), aryl(alkyl), heterocyclyl(alkyl), etc.; R2 = H, OH; R4 = azolylamino, N-(azolylalkyl)carbamoyl; R5 = substituted amino] were prepd. Thus, Me2CHCHRNH2 (R = imidazol-2-yl) (prepn. given) was condensed with (2R, 4S, 5S)-PhCH2CH(NHCO2CMe3)CH(OR6)CH2CH(CH2Ph)COR7 (II; R6 = SiMe2CMe3, R7 = OH) to give, after deprotection, II (R6 = H, R7 = NHCHRCHMe2, R = imidazol-2-yl). I had Ki of 1 nM to 5 .mu.M for inhibition of HIV-1 protease.
IT **149356-57-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as retroviral protease inhibitor)
RN 149356-57-0 CAPLUS
CN Carbamic acid, [2-hydroxy-5-[[1-(1H-imidazol-2-yl)-2-methylpropyl]amino]-5-oxo-1,4-bis(phenylmethyl)pentyl]-, 1-(1H-imidazol-2-yl)-2-methylpropyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1992:152273 CAPLUS
DOCUMENT NUMBER: 116:152273
TITLE: Synthesis of a contiguous tricyclic purine system: entry to unique nucleosides
AUTHOR(S): Nair, Vasu; Purdy, David F.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Tetrahedron Letters (1991), 32(51), 7503-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A unique class of hypermodified purine nucleosides, e.g., I, where the carbohydrate moiety is fused to the imidazole ring, has been designed and synthesized regiospecifically and stereospecifically using a multi-step approach starting from 1-O-acetyl-2,3,5-tri-O-benzoyl-.beta.-D-ribofuranose and Me3SiNHC(CN):C(CN)NHSiMe3.

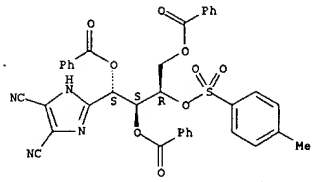
IT **139545-87-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and intramol. cyclocondensation of)

RN 139545-87-2 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 2-[1,2,4-tris(benzoyloxy)-3-[[(4-methylphenyl)sulfonyl]oxy]butyl]-, [1S-(1R*,2R*,3S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L13 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)

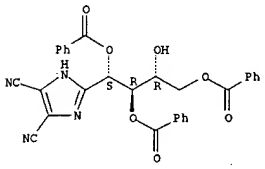


IT **101946-17-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and tosylation of)

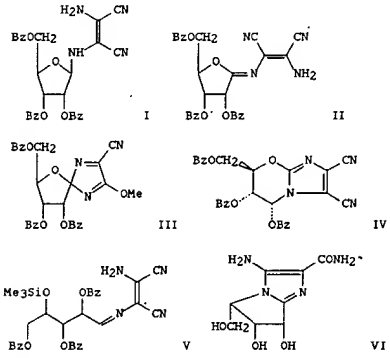
RN 101946-17-2 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 2-[1,2,4-tris(benzoyloxy)-3-hydroxybutyl]-, [1S-(1R*,2S*,3S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:459396 CAPLUS
DOCUMENT NUMBER: 107:59396
TITLE: Spiro and bicyclic nucleosides. Preparation of new structural types from ribose adducts of diaminomaleonitrile
AUTHOR(S): Ferris, James P.; Devadas, Balekudru
CORPORATE SOURCE: Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180-3590, USA
SOURCE: Journal of Organic Chemistry (1987), 52(12), 2355-61
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:59396
GI



I II III IV V VI

AB Three new nucleoside structural types were prepd. from ribose adducts of diaminomaleonitrile. Thus, oxidn. of adduct I with DDQ in MeCN and with DDQ in MeOH gave iminolactone II and spiro deriv. III, resp. Treatment of II with N-bromosuccinimide gave imidazooxazine IV. The acyclic adduct V was converted to pyrroloimidazole VI in 6 steps.

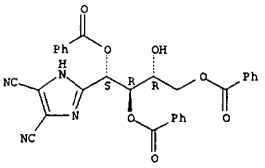
IT **101946-17-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reactions of)

RN 101946-17-2 CAPLUS

CN 1H-Imidazole-4,5-dicarbonitrile, 2-[1,2,4-tris(benzoyloxy)-3-hydroxybutyl]-, [1S-(1R*,2S*,3S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L13 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)

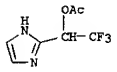


L13 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:626441 CAPLUS
DOCUMENT NUMBER: 105:226441
TITLE: Thermal condensation of imidazole with trifluoroacetaldehyde
AUTHOR(S): Fujii, Shozo; Maki, Yasuo; Kimoto, Hiroshi; Cohen, Louis A.
CORPORATE SOURCE: Gov. Ind. Res. Inst., Nagoya, 462, Japan
SOURCE: Journal of Fluorine Chemistry (1986), 30(4), 415-28
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:226441

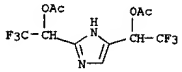
AB The condensation of imidazole with CF3CH(OH)OMe occurred readily at reflux to give 4-(1-hydroxy-2,2,2-trifluoroethyl)imidazole (37.3%), 2-(1-hydroxy-2,2,2-trifluoroethyl)imidazole (8.8%), 2,4-bis(1-hydroxy-2,2,2-trifluoroethyl)imidazole (7.2%), and 4,5-bis-product (0.4%). (Trifluoroacetyl)imidazoles were prepd. by oxidn. of these condensation products. Nitration and bromination of the condensation products gave the corresponding nitro- and bromoimidazoles, resp.

IT **105480-25-9P 105480-26-0P 105480-38-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 105480-25-9 CAPLUS
CN 1H-Imidazole-2-methanol, .alpha.-(trifluoromethyl)-, acetate (ester) (9CI) (CA INDEX NAME)

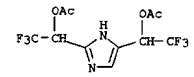


RN 105480-26-0 CAPLUS
CN 1H-Imidazole-2,4-dimethanol, .alpha.,.alpha.'-bis(trifluoromethyl)-, diacetate (ester), (R*,R*)- (9CI) (CA INDEX NAME)



RN 105480-38-4 CAPLUS
CN 1H-Imidazole-2,4-dimethanol, .alpha.,.alpha.'-bis(trifluoromethyl)-, diacetate (ester), (R*,S*)- (9CI) (CA INDEX NAME)

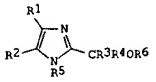
L13 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



L13 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:442804 CAPLUS
DOCUMENT NUMBER: 105:42804
TITLE: Antihypertensive 4,5-diaryl-1H-imidazole-2-methanol derivatives
INVENTOR(S): Wexler, Ruth R.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4576958	A	19860318	US 1984-573214	19840123

OTHER SOURCE(S): CASREACT 105:42804
GI

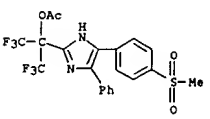


I

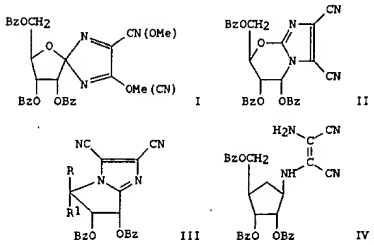
AB The antihypertensive title compds. I (R1, R2 = 3-pyridyl, 2-thienyl, (un)substituted Ph; R3, R4 = H, C1-3 alkyl, cyclopropyl, CF3, CHF2, etc.; R5, R6 = H, C1-3 alkyl, R7CO, CO2R7, R7 = C1-2 alkyl) and their salts, were prepd. Thus, I (R1 = Ph; R2 = 4-MeSC6H4; R3 = R4 = CF3; R5, R6 = H) prepd. in 6 steps from Friedel-Crafts acylation of PhSMe with PhCH2COCl, was oxidized with Oxone in MeOH to give I (R1 = Ph; R2 = MeSO2C6H4; R3 = R4 = CF3; R5, R6 = H) (II). The antihypertensive activity of II was demonstrated in normotensive unanesthetized dogs.

IT **103090-02-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as antihypertensive)

RN 103090-02-4 CAPLUS
CN 1H-Imidazole-2-methanol, 4-[4-(methylsulfonyl)phenyl]-5-phenyl-.alpha.,.alpha.-bis(trifluoromethyl)-, acetate (ester) (9CI) (CA INDEX NAME)



L13 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:207593 CAPLUS
DOCUMENT NUMBER: 104:207593
TITLE: The synthesis of spiro and bicyclic nucleosides from ribose adducts of diaminomaleonitrile
AUTHOR(S): Ferris, James P.; Devadas, Balekudru
CORPORATE SOURCE: Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12180-3590, USA
SOURCE: Tetrahedron Letters (1986), 27(3), 323-6
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:207593
GI



I II III IV

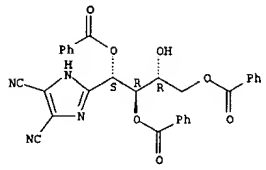
AB Spiro nucleoside I and bicyclic nucleosides II and III (R = H, R1 = B2OCH2; R = B2OCH2, R1 = H) were prepd. from the title adducts. For example, oxidn. of adduct IV with 2 equivs. of dichlorodicyanoquinone (DDQ) in MeOH resulted in 45% yield of one of the 2 possible regioisomers of I. Only 1 equiv. of DDQ was consumed when the oxidn. of IV was performed in MeCN to give a product (yield 50%) which on treatment with 1 equiv. of NBS at room temp. gave 55% II.

IT **101946-17-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and cyclization of)

RN 101946-17-2 CAPLUS
CN 1H-Imidazole-4,5-dicarbonitrile, 2-[1,2,4-tris(benzoyloxy)-3-hydroxybutyl]-, [1S-(1R*,2S*,3S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L13 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



L13 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:149615 CAPLUS
DOCUMENT NUMBER: 98:149615
TITLE: Antiinflammatory 4,5-diaryl-1H-imidazole-2-methanol
INVENTOR(S): Whitney, Joel G.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co. , USA
SOURCE: U.S., 12 pp. Cont.-in-part of U.S. Ser. No. 199,731, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4372964	A	19830208	US 1981-294747	19810820
DK 8005135	A	19810708	DK 1980-5135	19801202
AU 8165969	A1	19810716	AU 1981-65969	19810105
NO 8100021	A	19810708	NO 1981-21	19810106
ZA 8100065	A	19820825	ZA 1981-65	19810106
FI 8100033	A	19810708	FI 1981-33	19810107
JP 56118072	A2	19810916	JP 1981-512	19810107
ES 498364	A1	19820601	ES 1981-498364	19810107

PRIORITY APPLN. INFO.: US 1980-109923 19800107
US 1980-181991 19800828
US 1980-199731 19801030
US 1980-19923 19800107
OTHER SOURCE(S): CASREACT 98:149615
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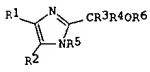
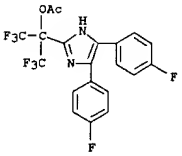


I

AB Analgesic and antiinflammatory compns. comprise I [R1 and R2 = Ph, substituted Ph, 3-pyridyl, or 2-thienyl; R3 and R4 = H, C1-3 alkyl, CF3, cyclopropyl, etc.; R5 = H or C1-3 alkyl; R6 = H, C1-3 alkyl, R7CO or CO2R7 (R7 = C1-2 alkyl)] and their salts. I (R5 and R6 = H) are prepd. by the treatment of the N-protected 4,5-disubstituted imidazole with BuLi in an inert solvent at low temp., followed by the addn. of aldehyde or ketone, and removal of the protecting group. Thus, a hard gelatin capsule contained active ingredient 50, lactose 175, talc 24, and Mg stearate 6 mg. In an adjuvant arthritis test in rats, the ED50 value of .alpha.-ethyl-4,5-bis(4-fluorophenyl)-.alpha.-(trifluoromethyl)-1H-imidazole-2-methanol (I; R1 and R2 = 4-FC6H4; R3 = CF3; R4 = Et; R5 and R6 = H) [85298-73-3] was 1.7 mg/kg.

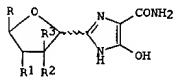
IT **85298-67-5P**
RL: PREP (Preparation)
(prepn. of, as analgesic and inflammation inhibitor)
RN 85298-67-5 CAPLUS
CN 1H-Imidazole-2-methanol, 4,5-bis(4-fluorophenyl)-.alpha.,.alpha.-

L13 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
bis(trifluoromethyl)-, acetate (ester) (9CI) (CA INDEX NAME)

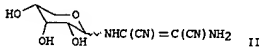


L13 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:462561 CAPLUS
DOCUMENT NUMBER: 95:62561
TITLE: General synthesis of imidazole C-nucleosides from carbohydrate adducts of diaminomaleonitrile
AUTHOR(S): Ferris, James P.; Badesha, Santokh S.; Ren, Wu Yun; Huang, Harry C.; Sorcek, Ronald J.
CORPORATE SOURCE: Dep. Chem., Rensselaer Polytech. Inst., Troy, NY, 12181, USA
SOURCE: Journal of the Chemical Society, Chemical Communications (1981), (3), 110-12
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

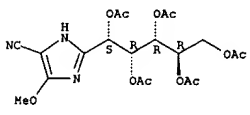


II

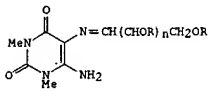
AB The imidazole C-nucleosides .alpha.- and .beta.-I (R = R3 = H, R1 = R2 = OH; R = CH2OH, R1 = R3 = OH, R2 = H) were prepd. from the adducts of ribose, arabinose, glucose, and mannose with diaminomaleonitrile. E.g., sequential treatment of the aminoribosylmaleonitrile II by DDQ (MeOH, room temp., 1.5 h), EtO(CH2)2OH-AcOH (150.degree., 3 h), Me2C(OMe)2, KOH-Me3COH, and Me3SiI gave .alpha.- and .beta.-I (R = R3 = H, R1 = R2 = OH).

IT **78300-58-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 78300-58-0 CAPLUS
CN D-Arabinitol, 1-C-(4-cyano-5-methoxy-1H-imidazol-2-yl)-, 1,2,3,4,5-pentaacetate, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:575651 CAPLUS
DOCUMENT NUMBER: 91:175651
TITLE: Studies on heterocyclic compounds. XXV. C-Glycosyl nucleoside. XI. Interaction of Schiff bases with metal halides in dimethyl sulfoxide
AUTHOR(S): Sakaguchi, Masakazu; Miyata, Yoshihisa; Ogura, Haruo; Gonda, Kinji; Koga, Shozo; Okamoto, Toshihiko
CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1979), 27(5), 1094-100
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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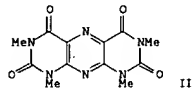
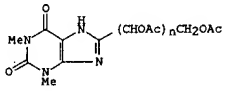


II

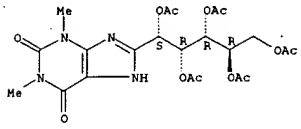


III

AB Reaction of Schiff bases I (R = H, n = 3-4), obtained from D-glucose, D-, and L-arabinose, with HgCl2 in Me2SO at room temp. gave pyrimidopteridine II quant. I (R = Ac, n = 3-4) on similar reaction gave 37-40% nucleoside analogs III. Similar Schiff bases of 5,6-diamino-1,3-dimethyluracil and (.+-.)-glyceraldehyde or PhCHO gave the corresponding theophylline or pteridine derivs. while H2NC(CN):C(CN)N:CHCH(OH)CH2OH gave 2,3-dicyano-5-methylpyrazine. PdCl2 instead of HgCl2 gave the corresponding products, but in low yields. MgCl2, CaCl2, BaCl2, SrCl2, ZnCl2, and CdCl2 gave no reaction with the Schiff bases.
IT **70497-18-6P 70497-19-7P 70518-84-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 70497-18-6 CAPLUS
CN D-Arabinitol, 1-C-(2,3,6,7-tetrahydro-1,3-dimethyl-6-oxo-1H-purin-8-yl)-, 1,2,3,4,5-pentaacetate, (S)- (9CI) (CA INDEX NAME)

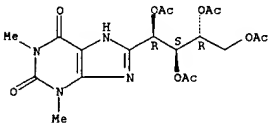
Absolute stereochemistry.

L13 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



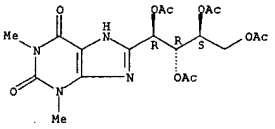
RN 70497-19-7 CAPLUS
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-[1,2,3,4-tetrakis(acetyloxy)butyl]-, [1R-(1R*,2S*,3R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

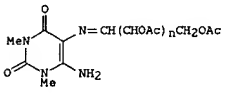


RN 70518-84-2 CAPLUS
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-[1,2,3,4-tetrakis(acetyloxy)butyl]-, [1R-(1R*,2R*,3S*)]- (9CI) (CA INDEX NAME)

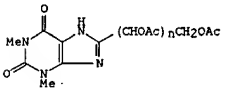
Absolute stereochemistry.



L13 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:439771 CAPLUS
DOCUMENT NUMBER: 91:39771
TITLE: C-Glycosyl nucleosides. XVII. A novel reaction of Schiff bases with mercuric chloride in dimethyl sulfoxide
AUTHOR(S): Ogura, Haruo; Sakaguchi, Masakazu; Okamoto, Toshihiko; Gonda, Kinji; Koga, Shozo
CORPORATE SOURCE: Sch. Pharm. Sci., Kitasato Univ., Tokyo, 108, Japan
SOURCE: Heterocycles (1979), 12(3), 359-63
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



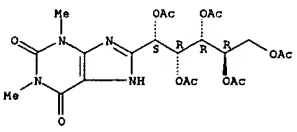
I



II

AB Pteridine or theophylline derivs. were obtained from the reaction of Schiff bases of 5,6-diamino-1,3-dimethyluracil with HgCl2 in Me2SO via radical or ionic mechanisms, which were confirmed by time dependent ESR and NMR spectra. Reactions of Schiff bases of D-glucose, D-, and L-arabinose (I; n = 4 or 3) with HgCl2 gave 35-40% theophylline nucleosides II.
IT **70497-18-6P 70497-19-7P 70518-84-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 70497-18-6 CAPLUS
CN D-Arabinitol, 1-C-(2,3,6,7-tetrahydro-1,3-dimethyl-6-oxo-1H-purin-8-yl)-, 1,2,3,4,5-pentaacetate, (S)- (9CI) (CA INDEX NAME)

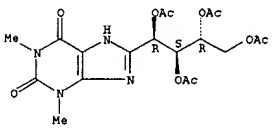
Absolute stereochemistry.



RN 70497-19-7 CAPLUS
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-[1,2,3,4-

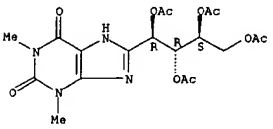
L13 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
tetrakis(acetyloxy)butyl]-, [1R-(1R*,2S*,3R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 70518-84-2 CAPLUS
CN 1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-8-[1,2,3,4-tetrakis(acetyloxy)butyl]-, [1R-(1R*,2R*,3S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



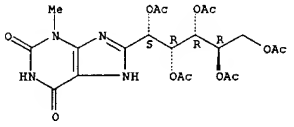
L13 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:87777 CAPLUS
DOCUMENT NUMBER: 90:87777
TITLE: Complex formation of nucleosides with mercury(II) chloride and cadmium chloride
AUTHOR(S): Gonda, Kinji; Koga, Shozo; Sakaguchi, Masakazu; Miyata, Yoshihisa; Ogura, Haruo; Okamoto, Toshihiko
CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, Japan
SOURCE: Yakugaku Zasshi (1978), 98(6), 708-14
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB From the NMR chem. shifts the formation consts. of 1:1 metal complexes with nucleosides were detd. in Me2SO at room temp. The complex formation consts. of CdCl2-adenine and CdCl2-benzyladenine are 1.6-1.7 times larger than the values for the HgCl2 complexes of adenine and benzyladenine. On the other hand, the formation const. of HgCl2-6-mercaptopurine is larger than the value of CdCl2-6-mercaptopurine. 6-Methylmercaptopurine did not complex with HgCl2 or CdCl2. In nucleosides, the complex formation const. with HgCl2 is in the order of 4-thiouridine, cyclocytidine, and cytidine. The complex formation with HgCl2 or CdCl2 was not obsd. with nucleoside analogs prepd. from 5,6-diamino-1-methyluracil with D-glucose or D-galactose.

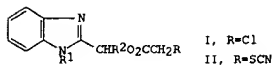
IT **69332-14-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and attempted complexation of, with mercuric chloride)

RN 69332-14-5 CAPLUS
CN D-Arabinitol, 1-C-(2,3,6,7-tetrahydro-3-methyl-2,6-dioxo-1H-purin-8-yl)-, 1,2,3,4,5-pentaacetate, (5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:468242 CAPLUS
DOCUMENT NUMBER: 87:68242
TITLE: Synthesis of thiocyanates derived from benzimidazole
AUTHOR(S): Sawlewicz, Jozef; Wisterowicz, Krystyna
CORPORATE SOURCE: Inst. Technol. Anal. Pharm. Prod., Sch. Med., Gdansk, Pol.
SOURCE: Acta Poloniae Pharmaceutica (1976), 33(4), 429-32
CODEN: APPHAX; ISSN: 0001-6837
DOCUMENT TYPE: Journal
LANGUAGE: Polish
GI

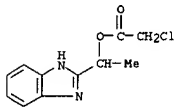


I, R=Cl
II, R=SCN

AB 2-(Hydroxymethyl)benzimidazole and ClCH2COCl in anhyd. dioxane yielded the benzimidazole I (R1 = R2 = H), which was treated with KSCN to give II (R1 = R2 = H). Analogously prepd. were I and II (R1 and R2 given): H, Me; Me, H; PhCH2, H; PhCH2, Me. Chloroacetylation of the N-substituted benzimidazoles required an excess of ClCH2COCl to be used. The benzimidazoles were bactericidal.

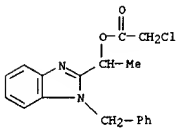
IT **62877-89-8P 62877-92-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with potassium thiocyanate)

RN 62877-89-8 CAPLUS
CN Acetic acid, chloro-, 1-(1H-benzimidazol-2-yl)ethyl ester (9CI) (CA INDEX NAME)



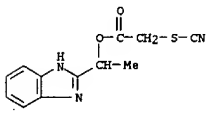
RN 62877-92-3 CAPLUS
CN Acetic acid, chloro-, 1-[1-(phenylmethyl)-1H-benzimidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)

L13 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)

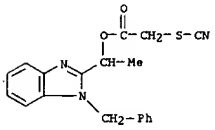


IT **62877-94-5P 62877-97-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

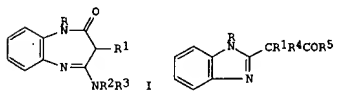
RN 62877-94-5 CAPLUS
CN Acetic acid, thiocyanato-, 1-(1H-benzimidazol-2-yl)ethyl ester (9CI) (CA INDEX NAME)



RN 62877-97-8 CAPLUS
CN Acetic acid, thiocyanato-, 1-[1-(phenylmethyl)-1H-benzimidazol-2-yl]ethyl ester (9CI) (CA INDEX NAME)



L13 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:171400 CAPLUS
DOCUMENT NUMBER: 86:171400
TITLE: Research on 1,5-benzodiazepines. I. Derivatives of 4-amino-1,5-benzodiazepine
AUTHOR(S): Roma, G.; Ermili, A.; Balbi, A.
CORPORATE SOURCE: Ist. Chim. Farm. Appl., Univ. Genova, Genoa, Italy
SOURCE: Farmaco, Edizione Scientifica (1977), 32(2), 81-91
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI

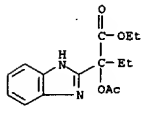


I II

AB Cyclocondensation of 2-H2NC6H4NHR (R = H, Ph) and EtO2CCHR1CONR2R3 (R1 = H, Me, Et; R2 = R3 = Me, Et; R2 = Me, Ph, R3 = Et; NR2R3 = pyrrolidino) in the presence of POCl3 gave benzodiazepines I. Also isolated from the reaction mixts. were benzimidazoles II (R = R1 = R4 = H, R5 = NEt2; R = H, R1 = Me, Et, R4 = OH, R5 = OEt; R = Ph, R1 = R4 = H, R5 = NMe2).

IT **62537-69-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 62537-69-3 CAPLUS
CN 1H-Benzimidazole-2-acetic acid, .alpha.-(acetyloxy)-.alpha.-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

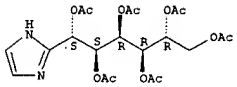


L13 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:520955 CAPLUS
DOCUMENT NUMBER: 81:120955
TITLE: Noncyclic c-nucleosides
INVENTOR(S): Matsui, Masanao; Ogawa, Tomoya; Yasui, Masayuki
PATENT ASSIGNEE(S): Institute of Physical and Chemical Research
SOURCE: Japan. Kokai, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49030361	A2	19740318	JP 1972-65630	19720630
JP 52003385	B4	19770127		

GI For diagram(s), see printed CA Issue.
AB Noncyclic C-nucleosides are prepd. by treating aldehydo sugars with 1-methyl-2-(trimethylsilyl)imidazole, 1,2-bis(trimethylsilyl)imidazole, 2-(trimethylsilyl)pyridine (I) or 2-lithiopyridine. Thus, 2.2 g 2,4:3,5-di-O-benzylidene-aldehydo-D-ribose was heated with 1.4 g I at 110.degree. for 3 hr, dissolved in aq. EtOH, and refluxed with a little pyridinium trifluoroacetate for 7 hr to give 72% 2-[2,4:3,5-di-O-benzylidene-D-altro-(and allo-)pentahydroxypentyl]pyridine (II), also prepd. in 77% yield with 2-lithiopyridine. Among 5 more C-nucleosides prepd. were 2-[2,4:3,5-di-O-benzylidene-D-altro-(and allo-)pentahydroxypentyl]imidazole, 1-methyl-2-[D-glycero-D-gulo-(and D-ido-)hexaacetoxyhexyl]imidazole, 2-[D-gl cero-D-gulo-(and D-ido-)hexaacetoxyhexyl]imidazole, and 2-[D-altro-(and D-allo-)pentaacetoxypentyl]imidazole.
IT **53428-61-8P 53428-62-9P 53428-63-0P 53428-64-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 53428-61-8 CAPLUS
CN D-Glucitol, 1-C-1H-imidazol-2-yl-, 1,2,3,4,5,6-hexaacetate, (S)- (9CI) (CA INDEX NAME)

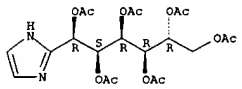
Absolute stereochemistry.



RN 53428-62-9 CAPLUS
CN D-Glucitol, 1-C-1H-imidazol-2-yl-, 1,2,3,4,5,6-hexaacetate, (R)- (9CI) (CA INDEX NAME)

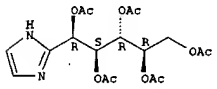
Absolute stereochemistry.

L13 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



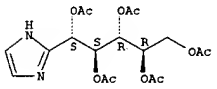
RN 53428-63-0 CAPLUS
CN D-Ribitol, 1-C-1H-imidazol-2-yl-, 1,2,3,4,5-pentaacetate, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

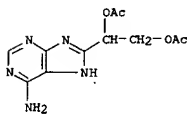


RN 53428-64-1 CAPLUS
CN D-Ribitol, 1-C-1H-imidazol-2-yl-, 1,2,3,4,5-pentaacetate, (S)- (9CI) (CA INDEX NAME)

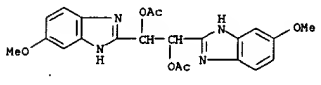
Absolute stereochemistry.



L13 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:449972 CAPLUS
DOCUMENT NUMBER: 81:49972
TITLE: Synthesis of 8-(hydroxyalkyl)adenines
AUTHOR(S): El Khadem, Hassan S.; Sindric, Ronald
CORPORATE SOURCE: Dep. Chem., Michigan Technol. Univ., Houghton, Mich., USA
SOURCE: Carbohyd. Res. (1974), 34(1), 203-7
CODEN: CRBRAT
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Condensation of 4,5,6-triaminopyrimidine with aldonic acids (glycolic, DL-glyeric, D-ribonic, D-xylonic, and D-allonic) gave amides that upon pyrolysis gave the title derivs. (I).
IT **53130-87-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 53130-87-3 CAPLUS
CN 1,2-Ethanediol, 1-(6-amino-1H-purin-8-yl)-, diacetate (ester) (9CI) (CA INDEX NAME)



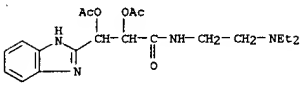
L13 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1972:470742 CAPLUS
DOCUMENT NUMBER: 77:70742
TITLE: Bisbenzimidazoles. Potent inhibitors of rhinoviruses
AUTHOR(S): Roderick, William R.; Nordeen, Carl W., Jr.; Von Esch, Anne M.; Appell, Raynor N.
CORPORATE SOURCE: Abbott Lab., North Chicago, Ill., USA
SOURCE: J. Med. Chem. (1972), 15(6), 655-8
CODEN: JMCMAR
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of 27 bisbenzimidazoles and 11 related monobenzimidazoles were prepd. by the method of Phillips (1928): condensation of a substituted o-phenylenediamine with a carboxylic acid in 5N HCl at 135.deg.. None of the monobenzimidazoles was active against rhinoviruses. The known (S,S)-1,2-bis(5-methoxy-2-benzimidazolyl)-1,2-ethanediol (Abbott 36683) (S,N-I) [34435-09-1] and 1,2-bis(5-methoxy-2-benzimidazolyl)ethane (II) [31253-05-1], (S)-1,2-bis(5-methoxy-2-benzimidazolyl)ethanol dihydrochloride hemihydrate (III.2HCl.0.5H2O) [35502-77-3], (R,R)-1,2-bis(5-methoxy-2-benzimidazolyl)-1,2-ethanediol (R,R-I) [34435-13-7], (S,S)-1,2-bis(5-ethoxy-2-benzimidazolyl)-1,2-ethanediol (S,S-IV) [34461-62-6] and S,S-I diacetate were active against rhinoviruses 1A and 42 in WI-38 cell culture at 10.mu.g/ml with S,S-I being the most active. Structural features essential for antiviral activity were: (1) no substituent on the 1 position of the benzimidazole; (2) a 5-methoxy or 5-ethoxy substituent; and (3) a 2-carbon chain, unsubstituted or substituted by hydroxyl, connecting the 2 benzimidazoles.
IT **37523-91-4**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(virucidal activity of)
RN 37523-91-4 CAPLUS
CN 1,2-Ethanediol, 1,2-bis(5-methoxy-1H-benzimidazol-2-yl)-, diacetate (ester), [S-(R*,R*)]- (9CI) (CA INDEX NAME)



L13 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1971:529812 CAPLUS
DOCUMENT NUMBER: 75:129812
TITLE: 4,5,6,7-Tetrahydrobenzimidazoles for use as corrosion inhibitors and antioxidants
INVENTOR(S): Butula, Ivan
PATENT ASSIGNEE(S): Rhein-Chemie Rheinau G.m.b.H.
SOURCE: Ger. Offen., 42 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

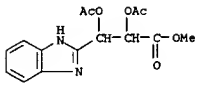
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1948795	A	19710408	DE 1969-1948795	19690926
GB 1310998	A	19730321	GB 1970-43850	19700914
JP 49024072	B4	19740620	JP 1970-83059	19700924
FR 2062636	A5	19710625	FR 1970-34761	19700925

PRIORITY APPLN. INFO.: DE 1969-1948795 19690926
GI For diagram(s), see printed CA Issue.
AB Substituted 4,5,6,7-tetrahydrobenzimidazoles I and their salts were prepd. by hydrogenation of the corresponding substituted benzimidazole in the presence of Rh or other suitable catalyst. For example, 2-(p-tert-butylphenyl)benzimidazole was hydrogenated at 120.degree. and 60 kg/cm2 over Rh/C to give 75% 2-(4-tert-butylcyclohexyl)-4,5,6,7-tetrahydrobenzimidazole (II). A vulcanizate prepd. from natural crepe rubber 100, ZnO 10, stearic acid 1, BaSO4 75, TiO2 10, S 3, diphenylguanidine 0.5, and II 2 parts was aged at 100.degree. for 48 hr and showed tensile strength and elongation values 121% and 60% greater, resp., than those of a vulcanizate contg. no II. The I were also used in lubricating oils to prevent the corrosion of Cu and Fe.
IT **26663-82-1P 26663-83-2P 26751-32-6P**
26785-90-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 26663-82-1 CAPLUS
CN 2-Benzimidazoleglyceramide, N-[2-(diethylamino)ethyl]-, diacetate (ester) (8CI) (CA INDEX NAME)

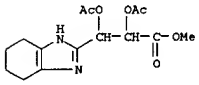


RN 26663-83-2 CAPLUS
CN 2-Benzimidazoleglyceric acid, methyl ester, diacetate (ester) (8CI) (CA INDEX NAME)

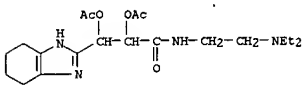
L13 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 26751-32-6 CAPLUS
CN 2-Benzimidazoleglyceric acid, 4,5,6,7-tetrahydro-, methyl ester, diacetate (ester) (8CI) (CA INDEX NAME)



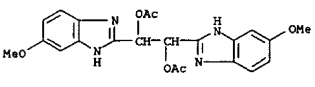
RN 26785-90-0 CAPLUS
CN 2-Benzimidazoleglyceramide, N-[2-(diethylamino)ethyl]-4,5,6,7-tetrahydro-, diacetate (ester) (8CI) (CA INDEX NAME)



L13 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1971:100046 CAPLUS
DOCUMENT NUMBER: 74:100046
TITLE: Antiviral 1,2-di-2-benzimidazolyl-1,2-ethanediols
INVENTOR(S): Shen, Tsung-Ying; Dorn, Coonrad P., Jr.; Grenda, Victor J.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Ger. Offen.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2038952	A	19710218	DE 1970-2038952	19700805
NL 7011010	A	19710209	NL 1970-11010	19700724
GB 1278566	A	19720621	GB 1970-1278566	19700804
FR 2068466	A5	19710827	FR 1970-28867	19700805

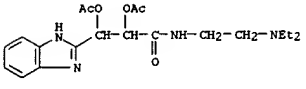
PRIORITY APPLN. INFO.: US 1969-848067 19690806
GI For diagram(s), see printed CA Issue.
AB The antiviral D, L, meso, and racemic forms of the title compds. (I) and (or) salts thereof were prepd. Thus, refluxing 4,2-MeO(H2N)C6H3-NHPr and L-tartaric acid in 4N HCl 18 hr yielded I.2HCl (R = MeO, R1 = R3 = R4 = H, R2 = Pr). Similarly prepd. were I (R4 = H) (R, R1, R2, R3, salt, and isomer given): MeO, H, H, Me, -, -; CO2H, H, H, H, 2HCl, -; MeO, MeO, H, H, 2HCl, -; CO2Et, H, H, H, 2HCl, -; F, H, H, H, 2HCl, L; MeS, H, H, H, 2HCl, L. I were converted by various methods (e.g., N-alkylation, O-acylation) into active I derivs.
IT **31545-10-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 31545-10-5 CAPLUS
CN 1,2-Ethanediol, 1,2-bis(5-methoxy-2-benzimidazolyl)-, diacetate (ester) (8CI) (CA INDEX NAME)



L13 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1970:111472 CAPLUS
DOCUMENT NUMBER: 72:111472
TITLE: 4,5,6,7-Tetrahydrobenzimidazole
INVENTOR(S): Butula, Ivan
PATENT ASSIGNEE(S): Rhein-Chemie G.m.b.H.
SOURCE: Ger. Offen., 43 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

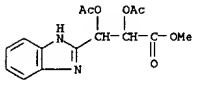
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1913184	A	19691002	DE 1969-1913184	19690314
GB 1260294	A	19720112	GB 1968-12750	19680315
FR 2003995	A5	19691114	FR 1969-7271	19690314
CH 520143	A	19720315	CH 1969-520143	19690314
US 3920678	A	19751118	US 1973-361106	19730517

PRIORITY APPLN. INFO.: GB 1968-12750 19680315
US 1969-807399 19690314
GI For diagram(s), see printed CA Issue.
AB Pd, Pd(OH)2, or a similar Pd compd. is used as the hydrogenation catalyst for the conversion of benzimidazoles to 4,5,6,7-tetra-hydrobenzimidazoles, without the simultaneous hydrogenation of other points of unsatn. in the benzimidazole mol. or in substituents (e.g., Ph groups) on the mol. The 4,5,6,7-tetrahydro-benzimidazoles are useful as corrosion inhibitors, antioxidants, chem. intermediates, epoxy resin hardeners, surfactants (as quaternary ammonium salts), etc. Thus, 1.2 g benzimidazole in 20 ml AcOH was hydrogenated during 18 min at 80.degree. under 1 atm H in the presence of 0.1 g Pd (on 1.9 g BaSO4) to give 4,5,6,7-tetrahydrobenzimidazole (I), m. 150.degree.. The reaction also proceeded readily in MeOH, 2N aq. HCl, 5.5% aq. HClO4, and similar solvents.
IT **26663-82-1P 26663-83-2P 26751-32-6P**
26785-90-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 26663-82-1 CAPLUS
CN 2-Benzimidazoleglyceramide, N-[2-(diethylamino)ethyl]-, diacetate (ester) (8CI) (CA INDEX NAME)

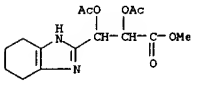


RN 26663-83-2 CAPLUS
CN 2-Benzimidazoleglyceric acid, methyl ester, diacetate (ester) (8CI) (CA INDEX NAME)

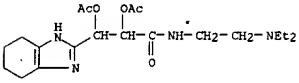
L13 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



RN 26751-32-6 CAPLUS
CN 2-Benzimidazoleglyceric acid, 4,5,6,7-tetrahydro-, methyl ester, diacetate (ester) (8CI) (CA INDEX NAME)



RN 26785-90-0 CAPLUS
CN 2-Benzimidazoleglyceramide, N-[2-(diethylamino)ethyl]-4,5,6,7-tetrahydro-, diacetate (ester) (8CI) (CA INDEX NAME)



L13 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:78285 CAPLUS
DOCUMENT NUMBER: 68:78285
TITLE: Carbamates of 2-(hydroxyalkyl)benzimidazoles
INVENTOR(S): Bywater, William G.; Brown, Bernard Beau; Clegg, John M.
PATENT ASSIGNEE(S): Penick, S. B., and Co.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3318889		19670509	US	19631014

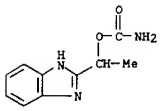
GI For diagram(s), see printed CA Issue.

AB The title compds. (I) are prepd. by treatment of an o-phenylenediamine with an appropriate hydroxy carboxylic acid, and conversion of the hydroxyalkylbenzimidazole thus formed to the carbamate by standard methods. Thus, a mixt. of 0.5 mole 4,5-dichloro-o-phenylenediamine and 0.75 mole glycolic acid was refluxed for 4-6 hrs. in a soln. of 400 ml. concd. HCl and 400 ml. H2O to yield 82.3% 5,6-dichloro-2-hydroxymethylbenzimidazole (II), m. 270-1.degree. (decompn.) (MeOH). II(0.03 mole) was dissolved in 75 ml. dry pyridine at 70.degree., the soln. cooled to 40.degree. with stirring, 0.0475 mole Me isocyanate added, and the mixt. kept at 70.degree. for 30 min. to give 46% 5,6-dichloro-2-(N-methylcarbamoyloxymethyl)benzimidazole (III), m. 225.degree. (decompn.). Alternatively, 0.06 mole Me2NCOCl was added to 0.05 mole II dissolved in 150 ml. dry pyridine and the mixt. refluxed for 4 hrs. to give 45% 4,5-dichloro - 2 - (N,N - dimethylcarbamoyloxymethyl)benzimidazole (IV), m. 176-8.degree.. In another method, a mixt. consisting of 0.5 mole 2-(.alpha.-hydroxyethyl)benzimidazole, 0.55 mole urethane, and a catalytic amt. of (iso-PrO)3Al was refluxed in toluene for 32 hrs. during which time 5 addnl. 2-3-g. portions of (iso-PrO)3Al were added to give 11.5 g. 2-(.alpha.-carbamoyloxyethyl)benzimidazole (V), m. 207-7.5.degree.. Other I prepd. by these methods were: 5,6-dichloro-2-(.beta.-N-methylcarbamoyloxyethyl)benzimidazole, m. 147-53.degree. (decompn.); 5,6-dichloro-2-(.gamma.-N-methylcarbamoyloxypropyl)benzimidazole, m. 178-80.degree.; 5,6-dichloro-2-(N-ethylcarbamoyloxymethyl)benzimidazole (VI), m. 225-7.degree.; 5,6-dichloro-2-(.alpha.-N-methylcarbamoyloxybenzyl)benzimidazole (VII), m. 157-8.degree. (decompn.); 5,6-dichloro-2-(.alpha.-N-ethylcarbamoyloxybenzyl)-benzimidazole, m. 171-3.degree.; 2-(N-methylcarbamoyloxymethyl)-benzimidazole, m. 120-1.degree.; 2-(.alpha.-N-methylcarbamoyloxyethyl)-benzimidazole, m. 110-11.degree.; 5(6)-chloro-2-(N-methylcarbamoyloxymethyl)benzimidazole, m. 99-100.degree.; 5(6)-chloro-2-(.alpha.-N-methylcarbamoyloxyethyl)benzimidazole, m. 203-5.degree.; 5(6)-nitro-2(N-methylcarbamoyloxymethyl)benzimidazole, m. 199-201.degree.. Quaternizations of I were carried out as follows. Equimolar amts. of IV and 4-amino-5-bromomethyl-2-propylpyrimidine dihydrobromide (VIII) were dissolved in MeOH and an equal vol. of MeCN was added to give 50% 3-(4-amino-2-propyl-5-pyrimidinylmethyl) - 5,6 - dichloro - 2 - (N,N - dimethylcarbamoyloxymethyl)benzimidazolium bromide dihydrobromide, m. 270.degree. (charring). Quaternary salts were prepd. from VIII and the

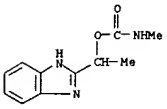
L13 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)
following I: V, VI, m. 170-5.degree. (decompn.), and VII. I are active against cecal coccidiosis in poultry and accelerate or retard certain sleep-inducing drugs.

IT **17577-51-4P 17577-58-1P 28258-42-6P 28724-58-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 17577-51-4 CAPLUS
CN 2-Benzimidazolemethanol, .alpha.-methyl-, carbamate (ester) (8CI) (CA INDEX NAME)

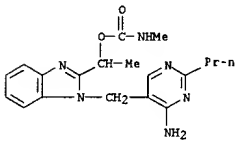


RN 17577-58-1 CAPLUS
CN Carbamic acid, methyl-, 1-(2-benzimidazolyl)ethyl ester (8CI) (CA INDEX NAME)



RN 28258-42-6 CAPLUS
CN Carbamic acid, methyl-, 1-[1-[(4-amino-2-propyl-5-pyrimidinyl)methyl]-5(or 6)-chloro-2-benzimidazolyl]ethyl ester, trihydrobromide (8CI) (CA INDEX NAME)

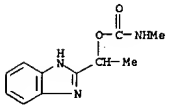
L13 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2002 ACS (Continued)



D1—Cl

●3 HBr

RN 28724-58-5 CAPLUS
CN Carbamic acid, methyl-, 1-(5-chloro-2-benzimidazolyl)ethyl ester (8CI) (CA INDEX NAME)



D1—Cl

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                                                       ENTRY    SESSION
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